Killer Apps: Neutrinos' Revenge

What makes a killer app?

- *Scientific Relevance*
- *Scale*
- *Complexity*
- *Benefit to Other Apps*

Anthony Mezzacappa (ORNL), SOS7, Durango, Colorado, March 5th, 2003

Two Classes of Supernovae:

Thermonuclear (Level I ASCI Flash Center)

Core Collapse (SciDAC TeraScale Supernova Initiative)

Explosions of Massive Stars

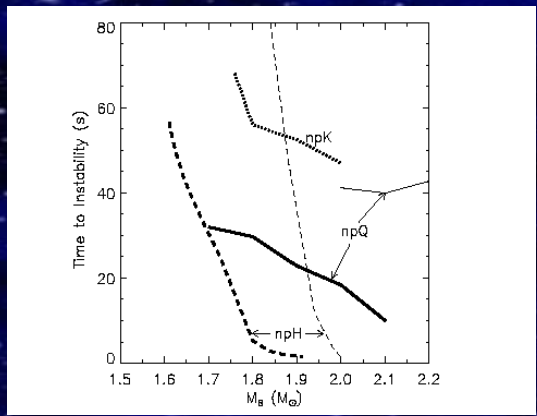
Relevance:

- ⇨Element Production
- ⇨Cosmic Laboratories
- ⇨Driving Application

H 1																	He 2
Li 3	Be 4											B 5	C 6	N 7	O 8	F 9	Ne 10
Na 11	Mg 12											Al 13	Si 14	P 15	S 16	Cl 17	Ar 18
K 19	Ca 20	Sc 21	Ti 22	V 23	Cr 24	Mn 25	Fe 26	Co 27	Ni 28	Cu 29	Zn 30	Ga 31	Ge 32	As 33	Se 34	Br 35	Kr 36
Rb 37	Sr 38	Y 39	Zr 40	Nb 41	Mo 42	Tc 43	Ru 44	Rh 45	Pd 46	Ag 47	Cd 48	In 49	Sn 50	Sb 51	Te 52	I 53	Xe 54
Cs 55	Ba 56	La 57	Hf 72	Ta 73	W 74	Re 75	Os 76	Ir 77	Pt 78	Au 79	Hg 80	Tl 81	Pb 82	Bi 83	Po 84	At 85	Rn 86
Fr 87	Ra 88	Ac 89	Rf 104	Db 105	Sg 106	Bh 107	Hs 108	Mt 109	Uun 110								

Ce 58	Pr 59	Nd 60	Pm 61	Sm 62	Eu 63	Gd 64	Tb 65	Dy 66	Ho 67	Er 68	Tm 69	Yb 70	Lu 71
Th 90	Pa 91	U 92	Np 93	Pu 94	Am 95	Cm 96	Bk 97	Cf 98	Es 99	Fm 100	Md 101	No 102	Lr 103

E.G.: Neutrino signal can tell us about high density composition.



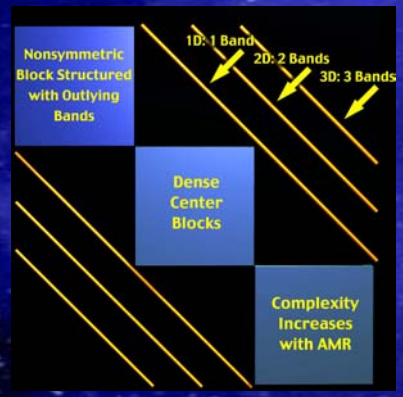
- ⇨*3D, multifrequency, multiangle precision radiation transport.*
- ⇨*Nuclear science (nuclear structure, …).*
- ⇨*Algorithms for large sparse linear system solution.*
- ⇨*Data management.*
- ⇨*Networking.*
- ⇨*Data analysis.*
- ⇨*Visualization.*
- ⇨*Software engineering.*

What will it take?

- Tera/Peta-Scale 3D, General Relativistic, Radiation Magnetohydrodynamics
- State of the Art Nuclear and Weak Interaction Physics

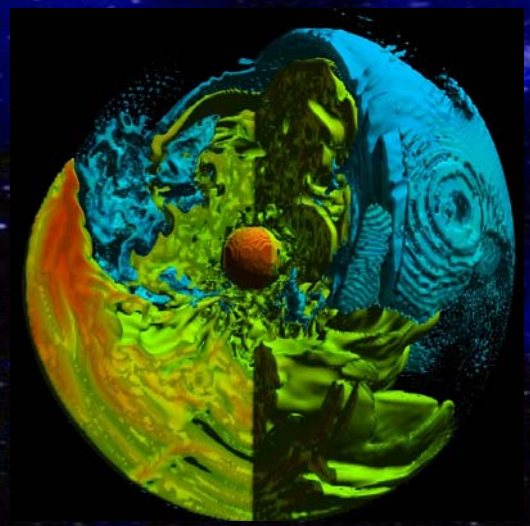
"Infrastructure" Needs: Transport

- Tera- and Peta-Scale Sparse Linear Systems of Equations



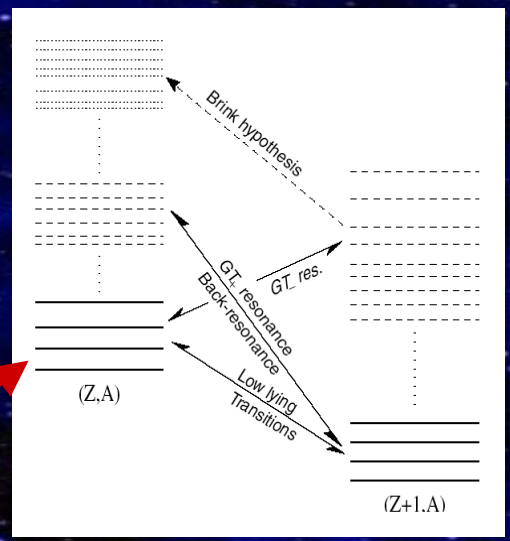
"Infrastructure" Needs: Hydrodynamics

- 1Gb/Write, 1-10 Tb/Variable/Simulation!
  - ➲ Manage?
  - ➲ Analyze?
  - ➲ Render?



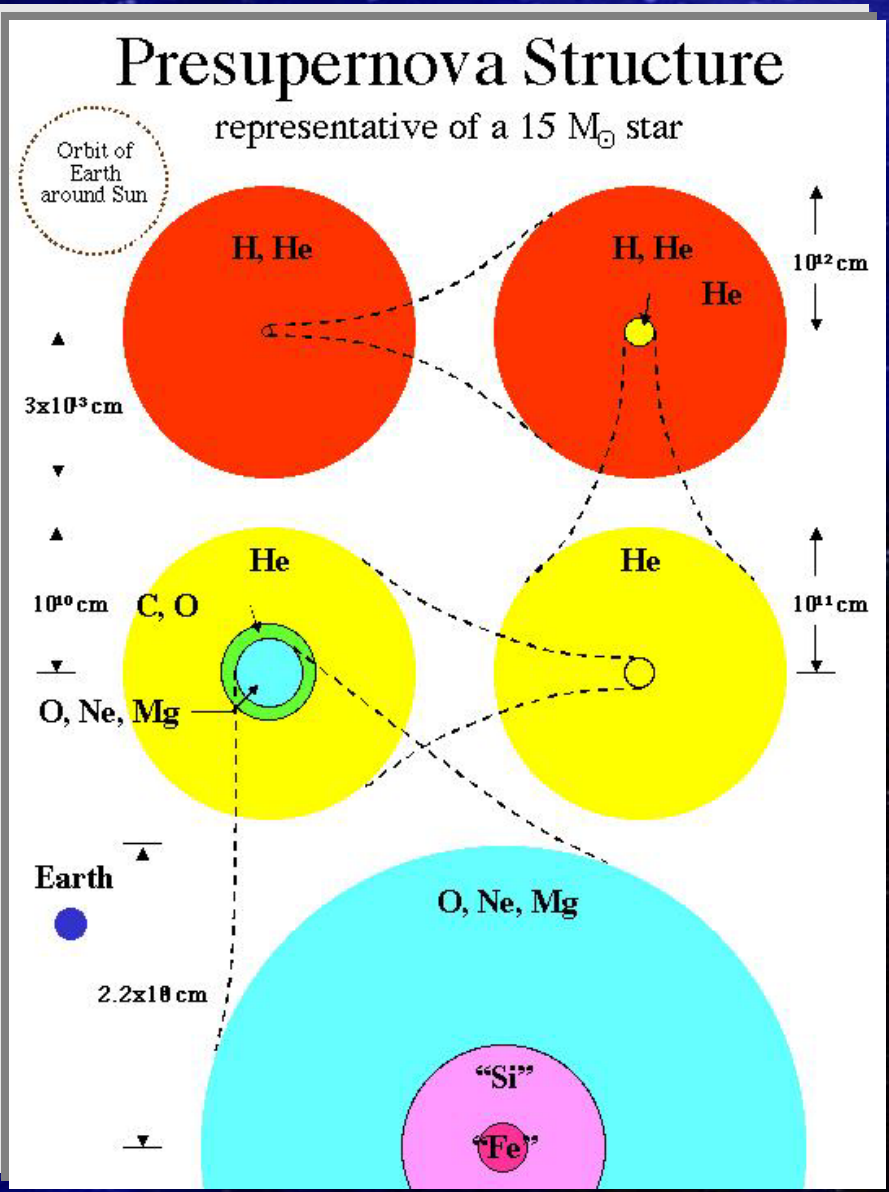
"Infrastructure" Needs: Weak Interactions

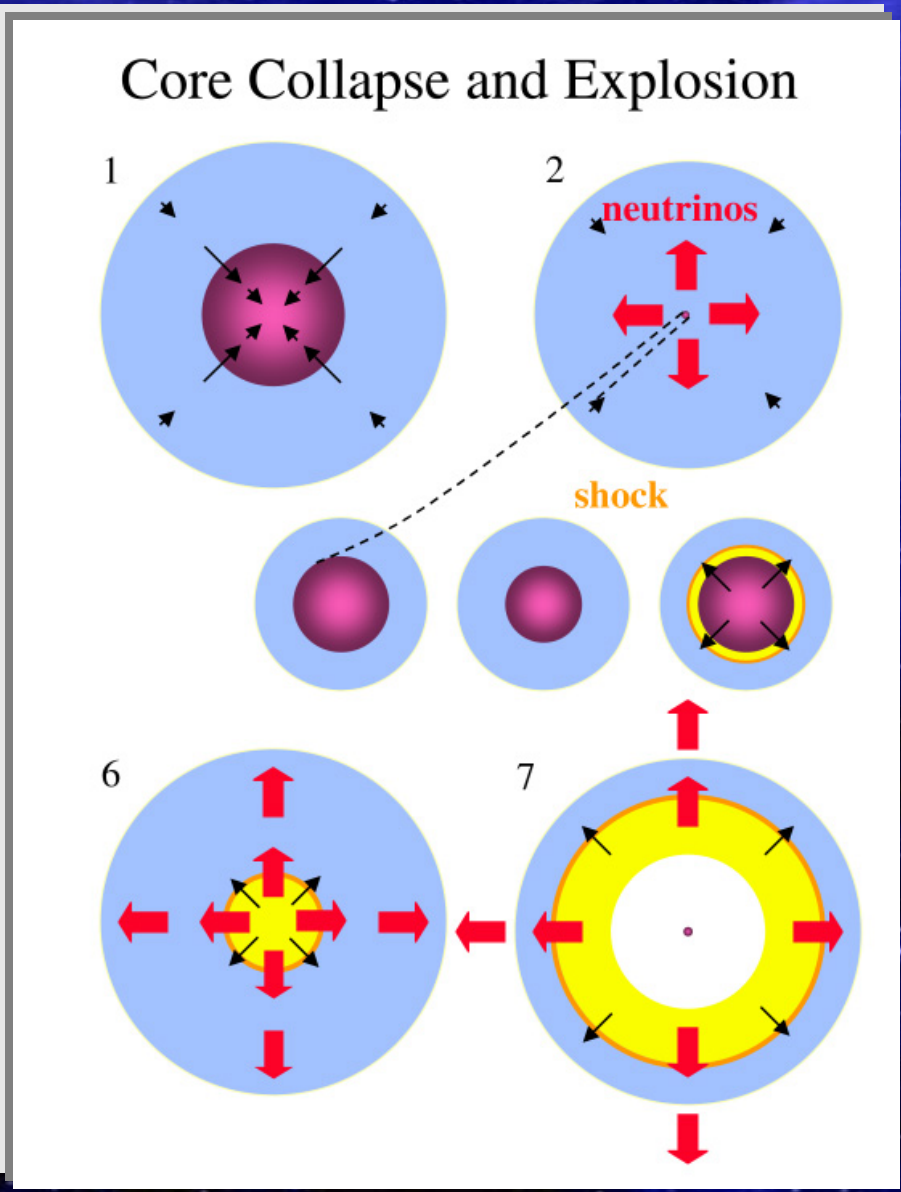
- TeraScale Nuclear "Structure" Computation



Nuclear Levels

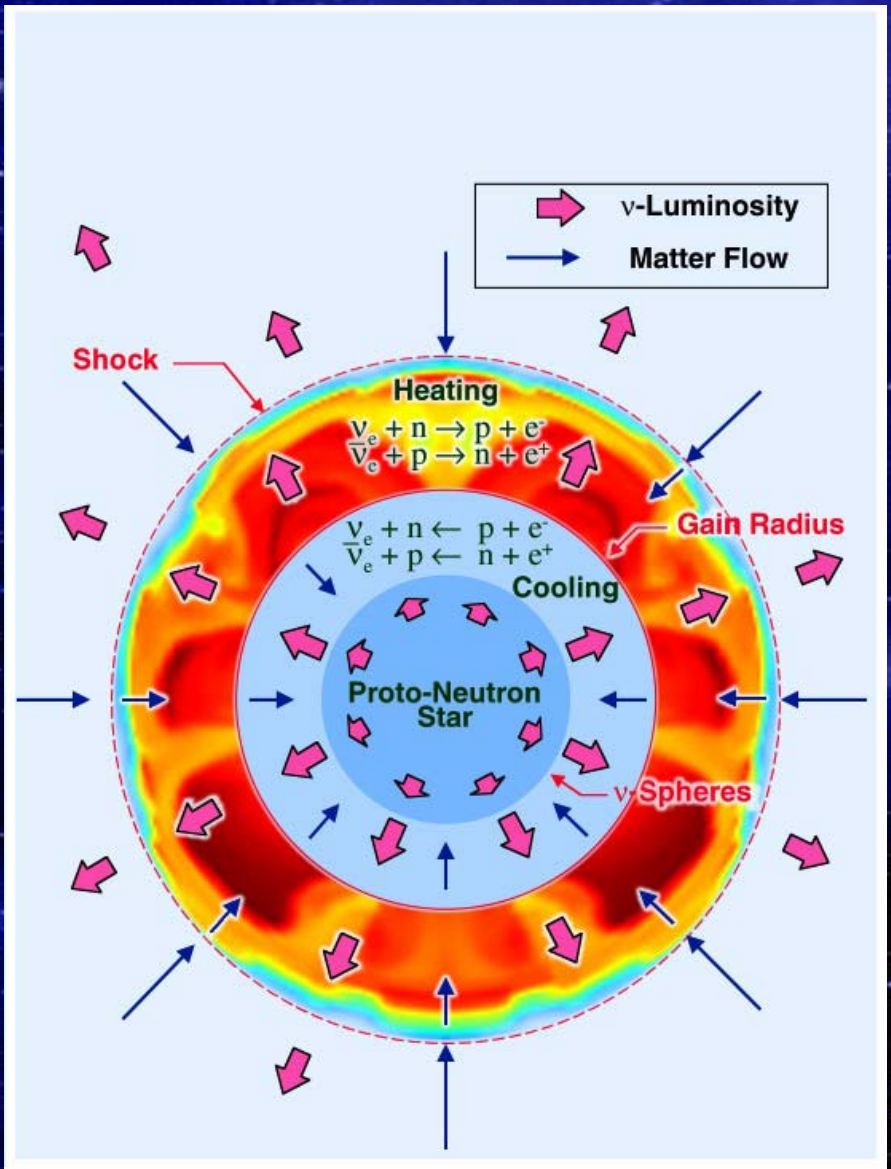
Core Collapse Paradigm

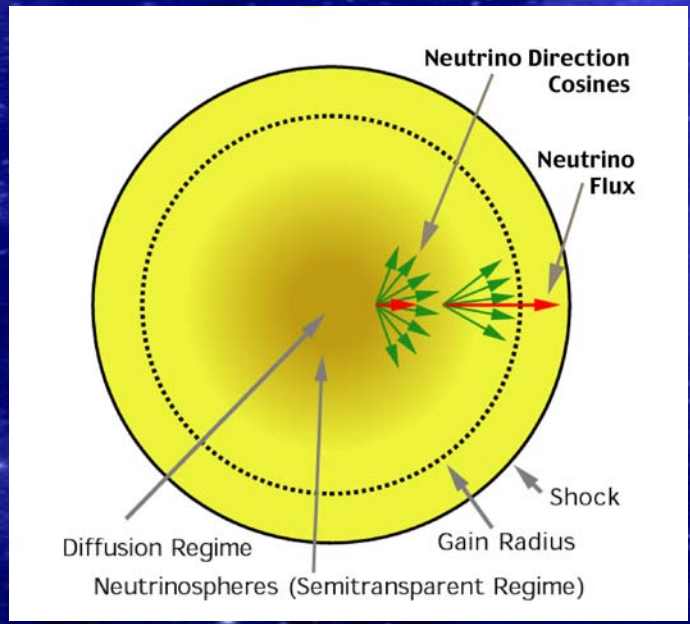




Anatomy of a Supernova

Convection





$$\dot{\epsilon} = \frac{X_n}{\lambda_0^a}\frac{L_{\nu_e}}{4\pi r^2}\langle E_{\nu_e}^2\rangle\left\langle\frac{1}{\mathcal{F}}\right\rangle + \frac{X_p}{\bar{\lambda}_0^a}\frac{L_{\bar{\nu}_e}}{4\pi r^2}\langle E_{\bar{\nu}_e}^2\rangle\left\langle\frac{1}{\bar{\mathcal{F}}}\right\rangle$$

- ***Need Boltzmann Solution***
  - ⇨ **Need Angular Distribution**
  - ⇨ **Need Spectrum**


QuickTime™ and a
Compact Video decompressor
are needed to see this picture.

Equations We Solve

Dominant Computation:
Nonlinear, integro-partial differential equations for the radiation distribution functions.

Spherical Symmetry	$f(r,\mu,E)$	$R(r,\mu,E,\mu',E')$
Axisymmetry	$f(r,\theta,\mu_1,\mu_2,E)$	$R(r,\theta,\mu_1,\mu_2,E,\mu_1',\mu_2',E')$
No Symmetry	$f(x,y,z,\mu_1,\mu_2,E)$	$R(x,y,z,\mu_1,\mu_2,E,\mu_1',\mu_2',E')$

Example: Boltzmann transport equation for spherical symmetry.

$$
\begin{aligned}
&\frac{1}{c}\frac{\partial F}{\partial t} + 4\pi\mu_0\frac{\partial(r^2\rho_0 F)}{\partial m} \\
&\quad + \frac{1}{r}\frac{\partial[(1-\mu_0^2)F]}{\partial\mu_0} \\
&\quad + \frac{1}{c}(\frac{\partial ln\rho_0}{\partial t} + \frac{3v}{r})\frac{\partial[\mu_0(1-\mu_0^2)F]}{\partial\mu_0} \\
&\quad + \frac{1}{c}[\mu_0^2(\frac{\partial ln\rho_0}{\partial t} + \frac{3v}{r}) - \frac{v}{r}]\frac{1}{E_0^2}\frac{\partial(E_0^3F)}{\partial E_0} \\
&\quad = \frac{j}{\rho_0} - \tilde{\chi}F \\
&\quad + \frac{1}{c}\frac{1}{h^3c^3}E_0^2\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0)F(\mu_0',E_0) \\
&\quad - \frac{1}{c}\frac{1}{h^3c^3}E_0^2F\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0) \\
&\quad + \frac{1}{h^3c^4}(\frac{1}{\rho_0} - F(\mu_0,E_0))\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{in}(\mu_0,\mu_0',E_0,E_0')F(\mu_0',E_0') \\
&\quad - \frac{1}{h^3c^4}F(\mu_0,E_0)\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{out}(\mu_0,\mu_0',E_0,E_0')(\frac{1}{\rho_0} - F(\mu_0',E_0'))
\end{aligned}
$$

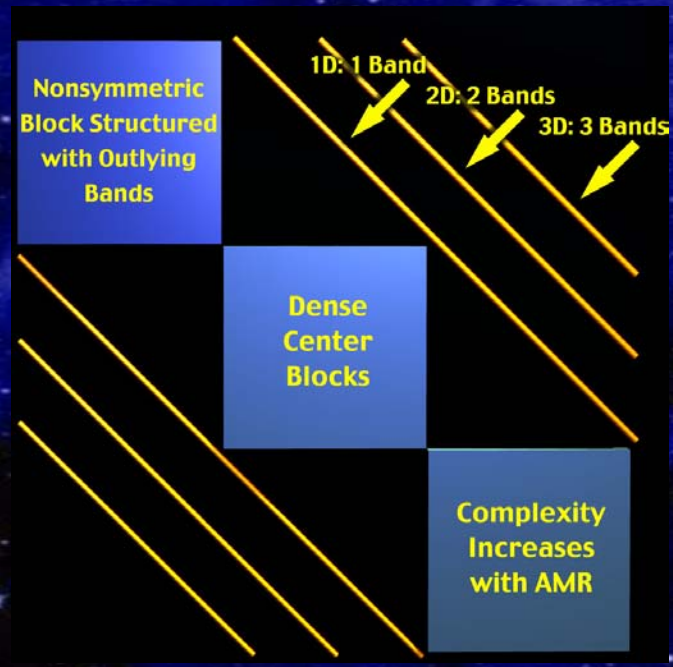
Large Sparse Linear System Solution

$$
\begin{aligned}
&\frac{1}{c}\frac{\partial F}{\partial t} + 4\pi\mu_0\frac{\partial(r^2\rho_0 F)}{\partial m} \\
&\quad + \frac{1}{r}\frac{\partial[(1-\mu_0^2)F]}{\partial\mu_0} \\
&\quad + \frac{1}{c}(\frac{\partial ln\rho_0}{\partial t} + \frac{3v}{r})\frac{\partial[\mu_0(1-\mu_0^2)F]}{\partial\mu_0} \\
&\quad + \frac{1}{c}[\mu_0^2(\frac{\partial ln\rho_0}{\partial t} + \frac{3v}{r}) - \frac{v}{r}]\frac{1}{E_0^2}\frac{\partial(E_0^3F)}{\partial E_0} \\
&\quad = \frac{j}{\rho_0} - \tilde{\chi}F \\
&\quad + \frac{1}{c}\frac{1}{h^3c^3}E_0^2\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0)F(\mu_0',E_0) \\
&\quad - \frac{1}{c}\frac{1}{h^3c^3}E_0^2F\int d\mu_0' R_{IS}(\mu_0,\mu_0',E_0) \\
&\quad + \frac{1}{h^3c^4}(\frac{1}{\rho_0} - F(\mu_0,E_0))\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{in}(\mu_0,\mu_0',E_0,E_0')F(\mu_0',E_0') \\
&\quad - \frac{1}{h^3c^4}F(\mu_0,E_0)\int dE_0' E_0'^2 d\mu_0' \tilde{R}_{NES}^{out}(\mu_0,\mu_0',E_0,E_0')(\frac{1}{\rho_0} - F(\mu_0',E_0'))
\end{aligned}
$$

Boltzmann Equation Nonlinear Integro-PDE

Nonlinear Algebraic Equations

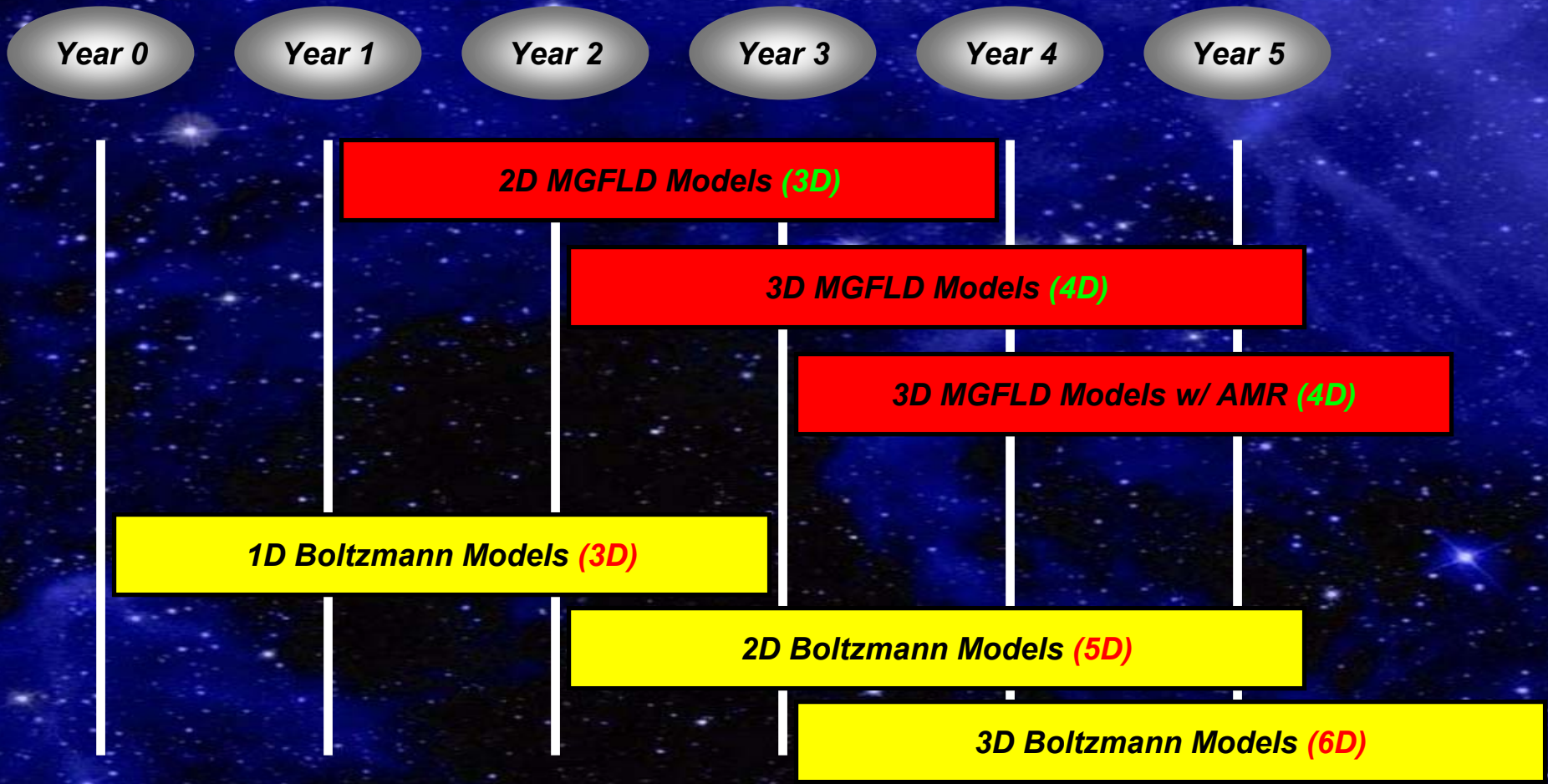
- *Linearize*
- *Solve via Multi-D Newton-Raphson Method*
  - ⇨ *Large Sparse Linear Systems*



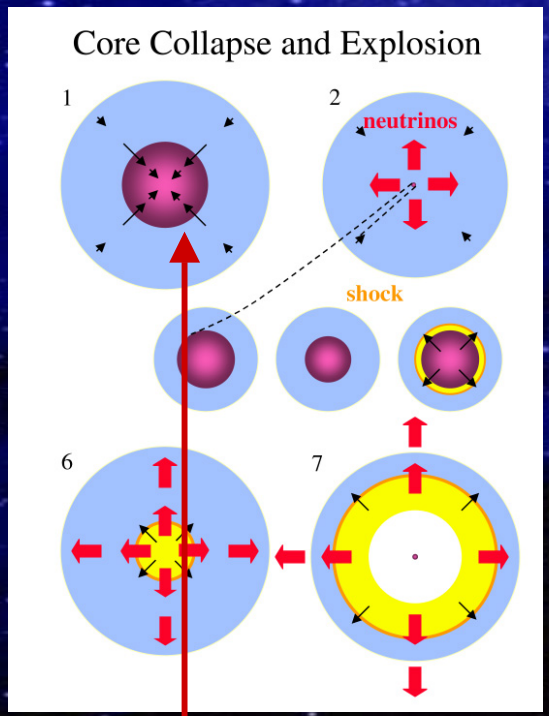
Implicit Time Differencing

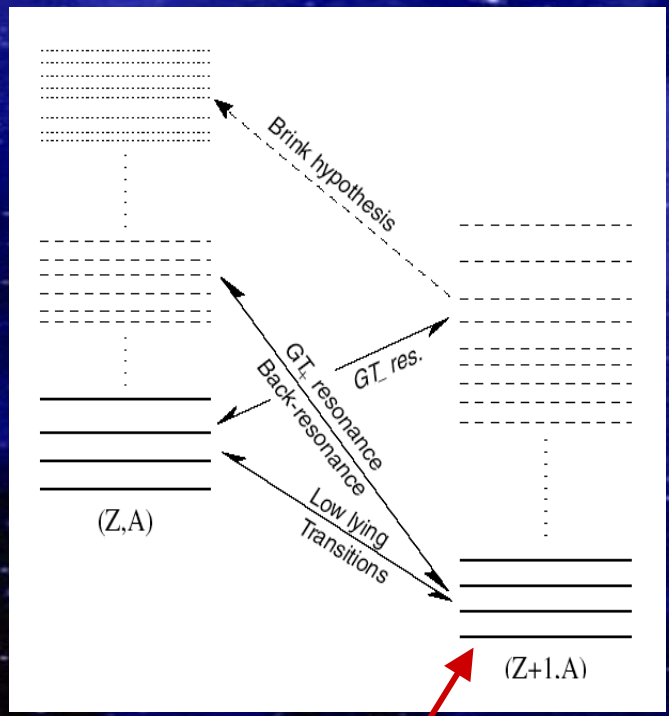
- *Extremely Short Neutrino-Matter Coupling Time Scales*
- *Neutrino-Matter Equilibration*
- *Neutrino Transport Time Scales*

Supernova Simulation Timeline



When Micro and Macro Worlds Meet...





⇨Size of inner core "piston" depends on total electron capture during collapse. Sets location of shock formation and initial shock energy.

⇨Nuclear electron capture rates depend on "structure" of nuclei in stellar core.

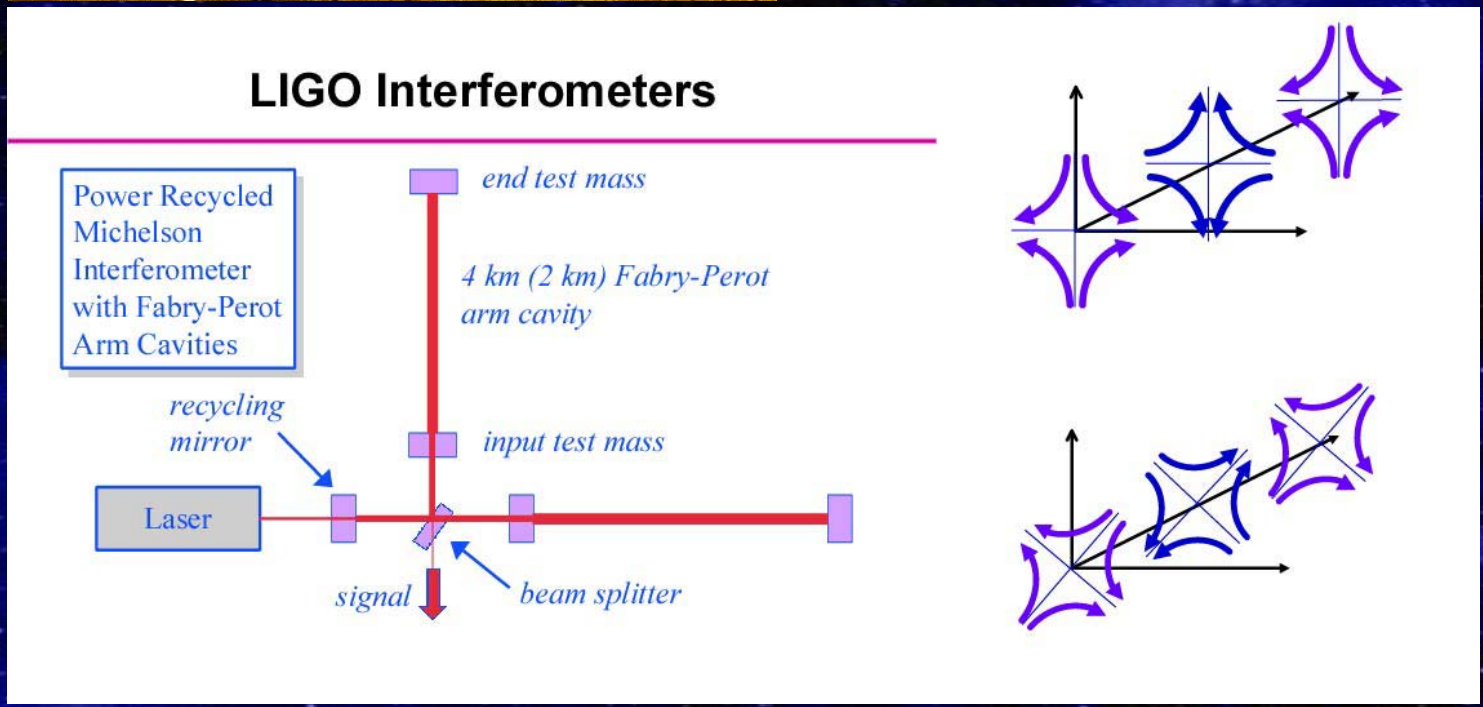
- Solve very large eigenvalue problems.

One of the most beautiful aspects of this problem!

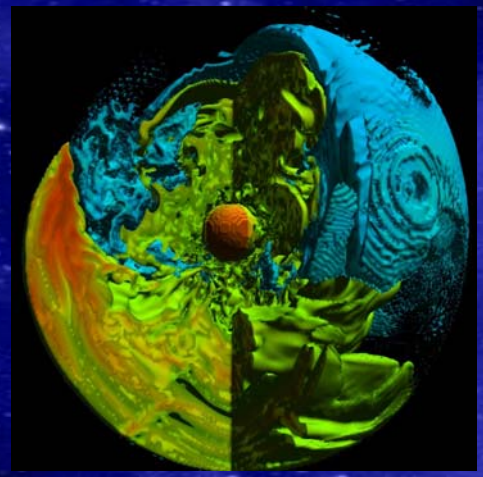
The "space" in which we live...

Gravitational Waves

- ⇨First direct evidence that spacetime is physical, a fabric, a participant.
- ⇨Core collapse supernovae are among the anticipated sources.
- ⇨LIGO would “see” a Galactic supernova.



Supernova Data



3D Hydrodynamics Run

- ⇨5 Variables (Density, Entropy, Three Fluid Velocities)
- ⇨1024 X 1024 X 1024 Cartesian Grid
- ⇨1000 Time Steps

→ ***20 Terabyte Dataset***

"The flea on the tail on the dog…"

Multidimensional Neutrino Data

$$f(x,y,z,\mu_1,\mu_2,E)$$

$$E_\nu(x,y,z,E)$$

$$F_\nu(x,y,z,E)$$

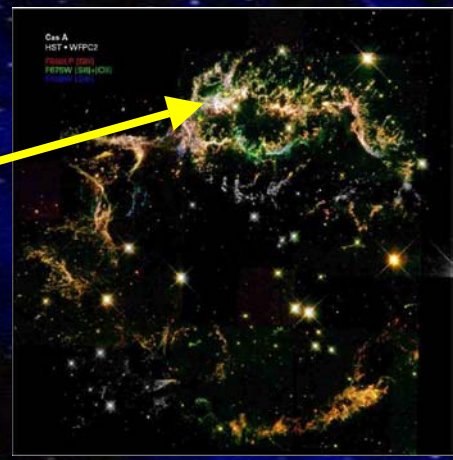
$$\frac{F_\nu(x,y,z,E)}{E_\nu(x,y,z,E)}$$

- ⇨Dataset Size!
- ⇨Custom Representations

Composition

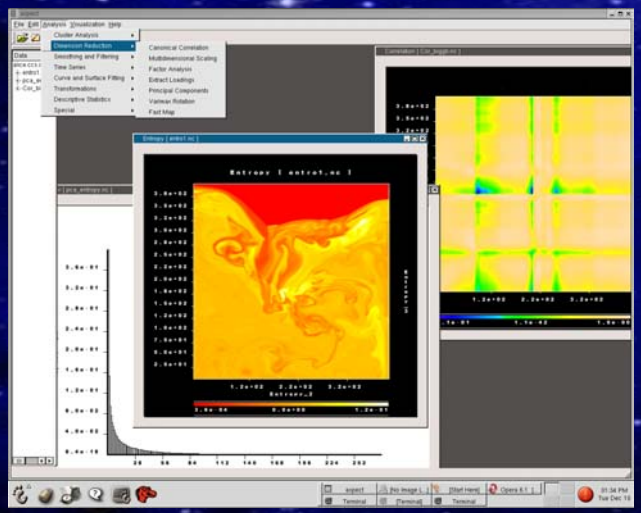
Query the composition of a fluid element.

Much of what we know about supernovae comes from light emitted from ejected atoms.



Driving developments in...

Samatova et al. (2002)



Data Reduction

Order of magnitude reduction using PCA techniques.

Data Analysis

Raw Data

Feature Extraction

Vortices, …

Feature-based visualization.

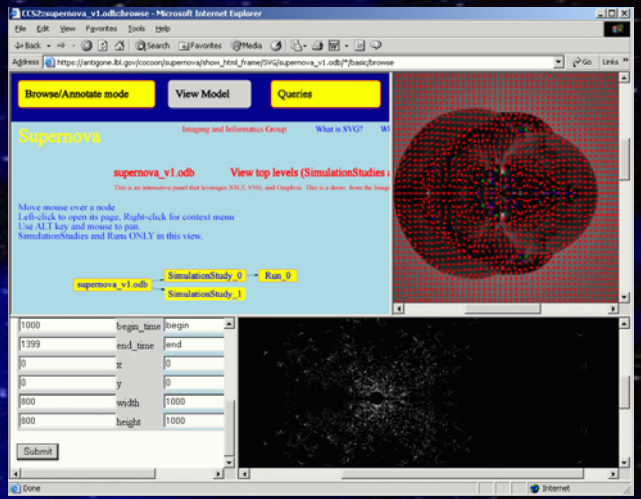
Dimensional Compression

Integration of Data Analysis and Visualization (ASPECT)

Agent Technology

Raised many issues.

Fontenay, Parvin (2002)



Reed, Potok (2002)

"QuickTime™ and a Cinepak decompressor are needed to see this picture."

…and networking and visualization (local, remote, collaborative)...

"Off-the-Shelf" Technologies

- ⇨EnSight
- ⇨TSB
- ⇨ParaView

QuickTime™ and a
Animation decompressor
are needed to see this picture.

Custom Visualization (VTK)

- ⇨Custom Representations
- ⇨Custom Functionality

Working with Logistical Networking and ORNL networking groups to significantly improve our data transfer rates between TSI "nodes" for local, remote, and collaborative visualization.

ORNL-NCSU Testbed

@220 Mbps

QuickTime™ and a
Animation decompressor
are needed to see this picture.

We are trying to understand our place in the Universe.
We must ultimately compute at the PetaScale.
We must worry about
- *3D hydrodynamics (esp. fluid instabilities, rotation),*
- *3D multifrequency, multiangle radiation transport,*
- *magnetic fields,*
- *as well as the structure of nuclei.*

We rely on developments in
- *discretizations of radiation transport,*
- *linear algebra,*
- *data management,*
- *data analysis,*
- *networking,*
- *visualization,*
- *performance optimization,*
- *and software engineering (esp. radiation hydrodynamics).*

Relevance
Scale
Complexity

Benefit
Other
Apps